REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

1. REPORT DATE (I	DD-MM-YYYY)	2. REPORT TYPE Technical Papers	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	2 DATE	S COVERED (From - To)
4 TITLE AND SUBT				3. DATE	,
	TITLE	recimical rapers		5a. CON	TRACT NUMBER
•					NIT KUISAN
		<	- 11 -	5b. GRA	INT NUMBER
	101	NAO	sel >	5c. PRO	GRAM ELEMENT NUMBER
			, 0.	\	S
AUTHOR(S)		- 1 -	1/1/10		JECT NUMBER
	\	afta		230	
					K NUMBER
				5f. WOR	C8 K UNIT NUMBER
				l	5709
PERFORMING O	RGANIZATION NAME	(S) AND ADDRESS(ES)		8. PERF	ORMING ORGANIZATION
in Found Dansons	h I ahanatamı (AENA	·C\		REPOR	T
ir Force Researc FRL/PRS	h Laboratory (AFM				
Pollux Drive					
lwards AFB CA	93524-7048				·
SPONSORING / N	MONITORING AGENO	Y NAME(S) AND ADDRE	ESS(ES)	10. SPO ACRON	NSOR/MONITOR'S
				AONON	T W(O)
	h Laboratory (AFM	(C)			
FRL/PRS					NSOR/MONITOR'S
Pollux Drive dwards AFB CA	03524 7049			NUM	IBER(S)
	/ AVAILABILITY STA			plea	se see attae
pproved for pub	lic release; distribut	ion unlimited			
approved for publ	ne release, distribut	ion ammitted.			
	RV NOTES	Party de la constantina della			
B. SUPPLEMENTA	111110120				
B. SUPPLEMENTA					
				A A A A A A A A A A A A A A A A A A A	
3. SUPPLEMENTA 4. ABSTRACT					
			^		
			21	1 03012	0 27/
			2(003012	9 234
			2(003012	9 234
			2(003012	9 234
. ABSTRACT			2(003012	9 234
I. ABSTRACT		·	2(003012	9 234
S. SUBJECT TERM	MS	·			
S. SUBJECT TERM			17. LIMITATION OF ABSTRACT	18. NUMBER 19a	9 234 a. NAME OF RESPONSIBLE RSON
S. SUBJECT TERM	MS		17. LIMITATION	18. NUMBER 198 OF PAGES PE	a. NAME OF RESPONSIBLE
4. ABSTRACT	MS	c. THIS PAGE	17. LIMITATION	18. NUMBER 198 OF PAGES PE Le	a. NAME OF RESPONSIBLE RSON

2303 M2C8

MEMORANDUM FOR PRS (In-House/Contractor Publication)

FROM: PROI (STINFO)

17 May 2002

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-VG-2002-118

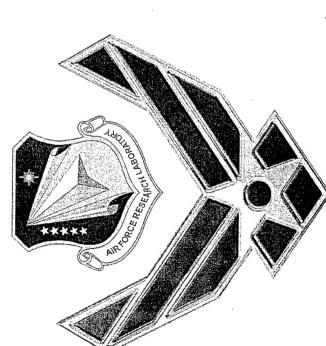
Jerry Boatz (PRSP) et al., "New Materials Design" (Viewgraphs)

DoD Users Group Conference (Austin, TX, 10-14 June 2002) (Deadline: 07 June 2002) (Statement A)

b.) military/national critical technology, c.) export cod.) appropriateness for release to a foreign nation, an	sclosure Office for: a.) appropriateness of distribution statemen ontrols or distribution restrictions, ad e.) technical sensitivity and/or economic sensitivity.
Signature	Date
	airs Office for: a.) appropriateness for public release
Signature	
Comments:	.) format and completion of meeting clearance form if required
Signature	Date
4. This request has been reviewed by PR for: a.) tech appropriateness of distribution statement, d.) technic national critical technology, and f.) data rights and particular technology.	al sensitivity and economic sensitivity, e.) military/ atentability
	APPROVED/APPROVED AS AMENDED/DISAPPROVED

PHILIP A. KESSEL Date
Technical Advisor
Space and Missile Propulsion Division

New Materials Design DoD UGC, 10-14 Jun 02 Austin, TX



Jerry Boatz Senior Research Chemist Air Force Research Laboratory

Propulsion Directorate



NEW MATERIALS DESIGN



THE TEAM....

Prof. Mark S. Gordon

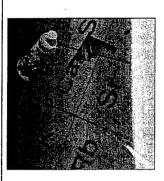
Prof. Gregory Voth



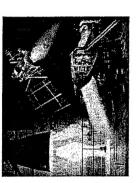
Prof. Sharon Hammes-Schiffer



Dr. Ruth Pachter, AFRL/MLPJ



Dr. Jerry Boatz, AFRL/PRSP



OUTLINE



1. Project Overview

- High energy density matter
- Polyhedral oligomeric silsesquioxanes (POSS)
- Non-linear optical materials

2. Theoretical Methods and benchmarks

- Ab initio electronic structure theory
- Nuclear-electronic orbital approach
- Centroid Molecular Dynamics

3. Results

4. Summary

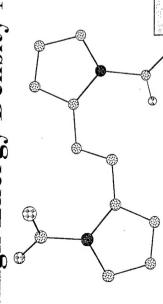




PROJECT OVERVIEW - HEDM



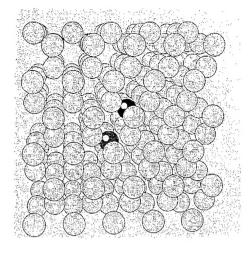
High Energy Density Matter -- next generation rocket propellants



High-nitrogen/polynitrogen compounds



Specific Impulse



Atom-doped solid hydrogen



PROJECT OVERVIEW - HEDM



Technical issues being addressed using CCM

1. High-nitrogen/polynitrogen compounds

Objective: identify, characterize, and synthesize stable compounds with high heats of formation, high densities

- structures, energy content, stabilities, reaction pathways

2. Energetic atoms in solid hydrogen

Objective: stabilize ~5% energetic atoms in solid hydrogen

stabilities, mobilities, concentration limits of atoms stored in hydrogen matrices

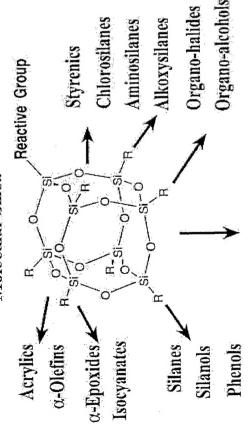


PROJECT OVERVIEW - POSS



Polyhedral oligomeric silsesquioxanes -- next generation plastics

Molecular Silica



Mechanical property/viscosity/thermal modifiers Heat/abrasion resistant paints and coatings Crosslinking agents Fire retardants

As Plastics

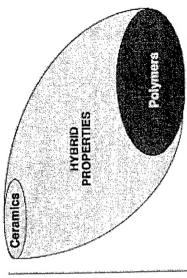
Space resistant resins Electronic materials Packaging/coatings Medical materials Optical Plastics

As Preceramics

Ablative materials (nozzles, insulations etc.) Precursors to glassy or ceramic matrices Claddings/electronics coatings

HYBRID POLYMERS

1.5 nm



Toughness

.5 nm

Temperature Ose



PROJECT OVERVIEW - POSS



Technical issues being addressed using CCM

1. Mechanisms of formation

Objective: rational design and synthesis of POSS

- role of solvents, acid/base catalysis, substituent effects on mechanism of formation

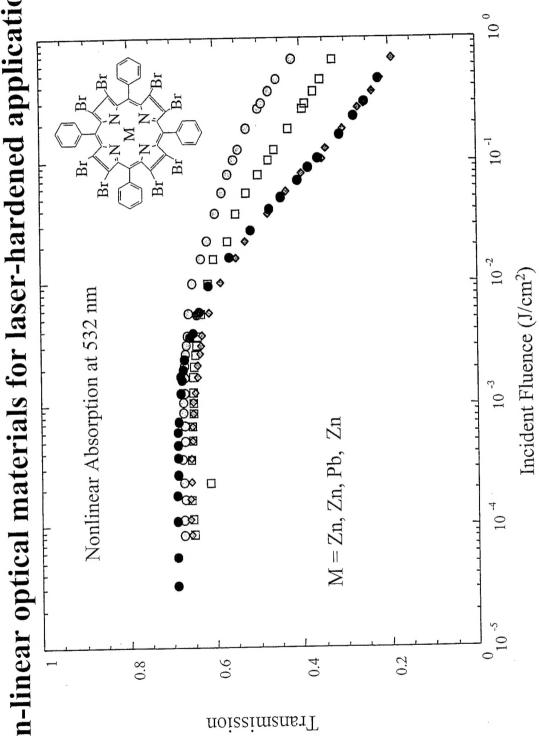
2. Potential applications as molecular "sieves"

Objective: determine if POSS cages can be used to separate small molecules

- determine barriers to encapsulation of N_2 and O_2

PROJECT OVERVIEW - NLO





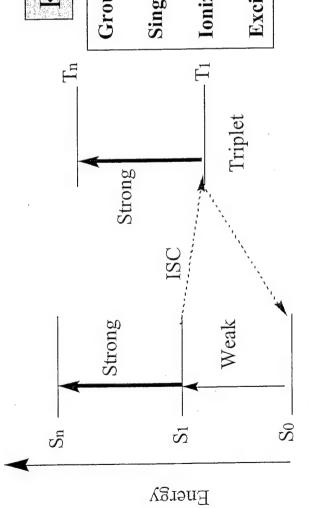


PROJECT OVERVIEW - NLO



Technical issues being addressed using CCM

1. Mechanism of reverse saturable absorption (RSA)



Key Components of RSA

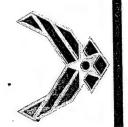
Ground state spectra (linear response)

Singlet-triplet splittings (ISC, phosphorescence)
Ionization potential (photoionization)

Excited triplet spectra (NLA)

Five-level model for nonlinear absorption

Singlet



PROJECT OVERVIEW - NLO

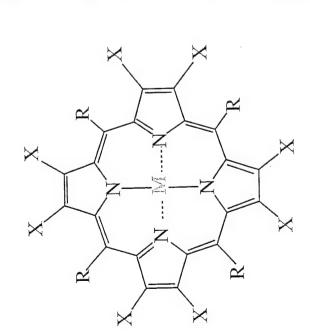


Technical issues being addressed using CCM

2. "Tuning" of absorption spectrum by benzannulation, halide substitution

Property

System



		×	×	IP	S_0 -Sn	S_0 - T_1	T_1 - T_n
PH_2		Н	H	E, C	E, C	E, C	E, C
ZnP		田	H	E, C	E, C	E, C	E, C
$TPPH_2$	The state of the s	H	0	E, C	E, C	E, C	E, C
ZnTPP	The state of the s	H	· •	E, C	E, C	E, C	E, C
ZnTPPBr8		Br	0	C	E, C	E, C	E, C

IP = Ionization Potential, S_0 - S_n = Ground State Spectrum, S_0 - T_1 = Singlet-Triplet Gap T_1 - T_n = Triplet-Triplet Spectrum E = Experiment, C = Calculated





1. Ab initio electronic structure theory

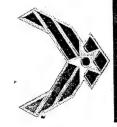
- General Atomic and Molecular Electronic Structure System (GAMESS) -- a CHSSI code
- Nuclear-electronic orbital approach (NEO) for including nuclear quantum effects (important, e.g., in proton transfer reactions)

molecular electronic Schrödinger equation from quantum mechanics: Various computational techniques are employed to solve the

$$-\frac{1}{2}\sum_{i}\nabla_{i}^{2} - \sum_{i}\sum_{\alpha}\frac{Z_{\alpha}}{r_{i\alpha}} + \sum_{i}\sum_{j>i}\frac{1}{r_{ij}}\left|\Psi_{el} = E_{el}\Psi_{el}\right|$$

Categories of approximate solutions:

- a) "Self-consistent field" (SCF): reasonably good geometries
- b) "Electron correlation": post-SCF correction, required for reliable energetics (e.g., barriers).





1. Ab initio electronic structure theory (cont.)

"clampled nuclei") approximation -- NOE method treats specified - Most electronic structure codes use Born-Oppenheimer (i.e., nuclei at QM level.

Nuclear-Electronic Hamiltonian

$$H_{\text{tot}}(\mathbf{r}_e, \mathbf{r}_q; \mathbf{r}_c) = -\sum_{i}^{N_e} \frac{1}{2} \nabla_i^2 - \sum_{i}^{N_e} \frac{Z_A}{A} + \sum_{i} \sum_{j>i}^{N_e} \frac{1}{r_{ij}}$$
$$-\sum_{i}^{N_p} \frac{1}{2M_I} \nabla_I^2 + \sum_{i}^{N_p} \sum_{N_c} \frac{Z_A Z_I}{A} + \sum_{i}^{N_p} \sum_{j>i}^{N_p} \frac{Z_I Z_J}{r_{IJ}}$$
$$-\sum_{i}^{N_e} \frac{1}{N_p} \sum_{i}^{N_c} \frac{Z_I}{A} + \sum_{i}^{N_c} \sum_{i}^{N_c} \frac{Z_A Z_B}{r_{AB}}$$
$$-\sum_{i}^{N_e} \sum_{I',i}^{N_p} \frac{Z_I}{I} + \sum_{i}^{N_c} \sum_{i}^{N_c} \frac{Z_A Z_B}{r_{AB}}$$

 N_e : number of electrons (coordinates ${\bf r}_e$) N_p : number of quantum nuclei (coordinates ${\bf r}_p$) N_c : number of classical nuclei (coordinates ${\bf r}_c$)





Ab initio electronic structure theory

Current Status of parallel GAMESS

	RHF	ROHF	뷤	GVB	MCSCF
Energy	dpo	cqb	cdp	cdp	cdp
Analytic Gradient	cdp	cdp	dpo	cqb	cdp
Numeric Hessian	dpo	cdp	cqb	cdp	dpo
Analytic Hessian	cdp	dpo	1	cdp	•
MP2 energy	cdp	dpo	дрэ	ı	c b
MP2 gradient	dpo		cq	1	1
CI energy	cqb	cqb		dpo	cqb
Cl gradient	cq	1		1	•
DFT energy	cdp	cdp	dpo	1	
DFT gradient	dpo	cdp	cdp		ı

c = conventional disk storage of AO integrals

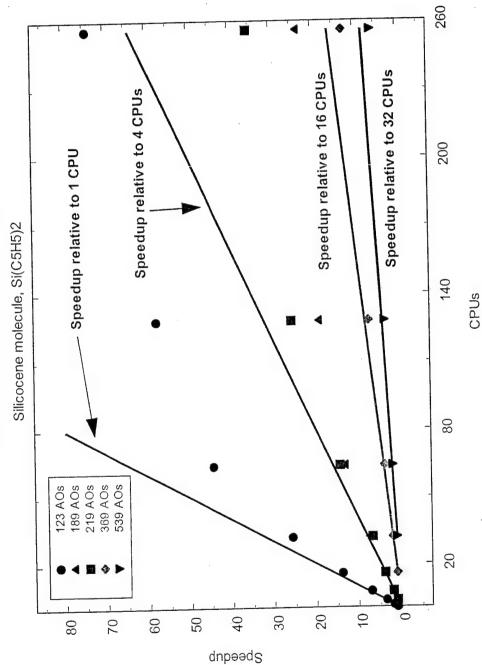
d = direct evaluation of AO integrals

p = runs in parallel



Ab initio electronic structure theory

MP2 Gradient Scalability Test





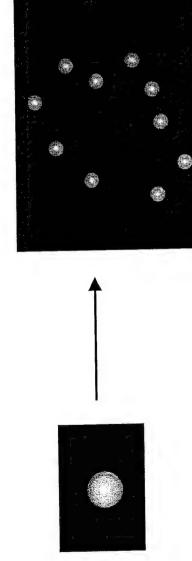


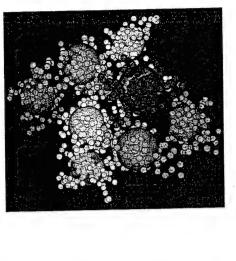




Path Integral Molecular Dynamics & Centroid Molecular Dynamics (CHSSI codes)

Simulation methods based on path integral techniques for mapping quantum particles onto "polymer ring" of classical quasiparticles:



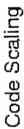


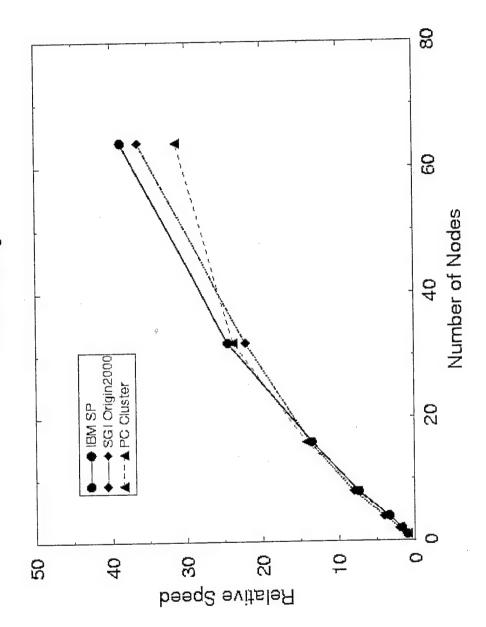
classical dynamics done on collection of quasiparticles => natural, Each "real" particle is replaced by N (50<N<500) quasiparticles; efficient parallelism.





Path Integral Molecular Dynamics & Centroid Molecular Dynamics







Input>rocket, chamber, 20.410000, exhaust, 0.010000

Rocket specific impulse calculation:

The chamber pressure = 20.41 atm The exhaust pressure = 0.01 atm

The initial equation error was huge: 24728.149173

The Chamber State:

 $\label{eq:Reference state} \mbox{Reference state = reactants} \\ \mbox{H(R)} = \mbox{H-1773.07}, \ \mbox{E(R)} = \mbox{E-1773.05}, \ \mbox{S(R)} = \mbox{S-0.00}$

S(R) VGS E(R) H(R) T P · V (CAL/GM) (CAL/K/GM) (CC/GM) (CAL/GM) (K) (CC/GM) (MTM) 2.389 909.6888 -449.64 0.00 909.6888 6436.6 20.4 1.)

Product concentrations

Name (mol/kg) (mol gas/mol explosive)

n2 Gas 2.112e+001 5.410e+000

co Gas 7.734e+000 1.981e+000

no Gas 4.609e+000 1.180e+000

o2 Gas 1.561e+000 3.998e-001

co2 Gas 7.513e-002 1.924e-002 no2 Gas 1.418e-003 3.632e-004

no2 Gas 1.418e-003 3.632e-004 *c solid 0.000e+000 0.000e+000

- --- 001 0 000-1000

Total Gas 3.510e+001 8.990e+000 Total Cond. 0.000e+000 0.000e+000

The Exhaust State:

Reference state = reactants H(R) = H-1773.07, E(R) = E-1773.05, S(R) = S-0.00

P V T H(R) E(R) S(R) VGS

(ATM) (CC/GM) (K) (CAL/GM) (CAL/GM) (CAL/K/GM) (CC/GM)

1.) 0.0 565350.1813 2148.9 -1863.53 -2000.43 2.389565350.1813

Product concentrations

Name (mol/kg) (mol gas/mol explosive)

n2 Gas 2.337e+001 5.984e+000

co2 Gas 6.157e+000 1.577e+000

co Gas 1.652e+000 4.232e-001 o2 Gas 7.645e-001 1.958e-001

o2 Gas 7.645e-001 1.958e-001 no Gas 1.234e-001 3.160e-002

no Gas 1.234e-001 3.160e-002 no2 Gas 5.283e-006 1.353e-006

*c solid 0.000e+000 0.000e+000

Total Gas 3.206e+001 8.212e+000

Total Cond. 0.000e+000 0.000e+000

The specific impulse = 402.54 seconds



RESULTS - HEDM



High-nitrogen/polynitrogen compounds

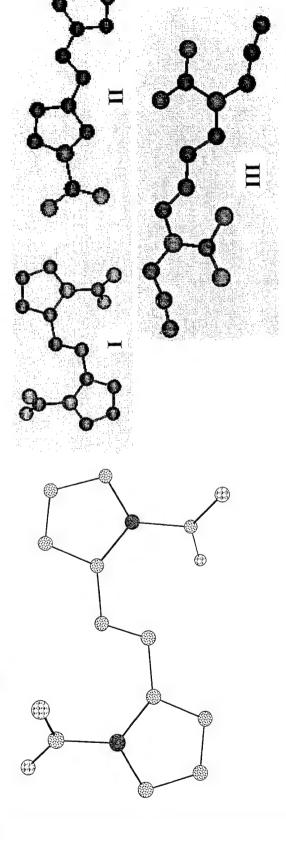
Predicted $\Delta H_f = 457 \text{ kcal/mol}$, $I_{sp} = 329 \text{ sec (sea level)}$

 $(I_{sp} \text{ for hydrazine} = 233 \text{ sec})$

Relative energies (kcal/mol)

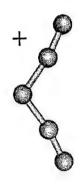
I: 0 II: -15

III: +36



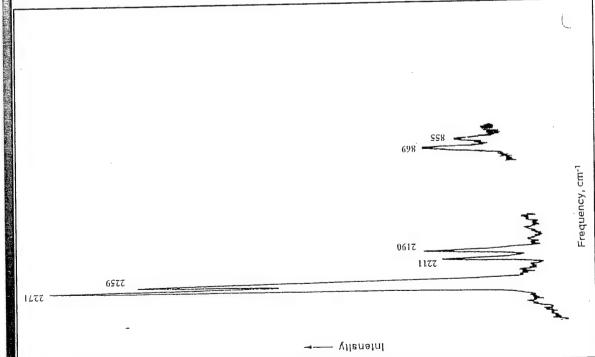
Computational requirements: 4500 MW memory, ~350,000 node-hrs, ERDC T3E

Comparison of Calculated and Measured Spectra Identifying a Completely New Molecule:



	0 9
	1 1 1
	S
_	
	4
- <i>II</i>	
(.)	
)	
77	
	N-14N and N-14N
X	1 - 10
	7
	15N14N14N14N14N]+AsF ₆ - and and 14N14N15N14N14N]+AsF ₆ -
	一门下海上的建筑中市 在外军中的影响

						Alk		
		Calc.t	~ ~ ~) 24.	Z 7.	$\overline{}$		
		ျ				4		
2		തി	7		$\mathbf{\Sigma}$	V		
		651			\mathcal{N}			S
)	\mathbf{C}						=
5. C412.								
ť	מ	i e						ဟ
*	5							O)
								_
	3							
		•						\sim
V	J	Obs.	, ,	1		4		61
		Ω			7			$\widetilde{\Box}$
	2	\cap						\cup
•	5							+
								$\overline{}$
7	J							$\overline{}$
38 . T	7				#\$K			က
	7							
	?							\mathfrak{S}
200								~
		(1)	-		\sim			\vdash
16		$\tilde{\sigma}$			\sim	σ		\asymp
-		Mode		<i>(LD)</i>	$v_7(b_2)$	(n)		tCCSD(T)/6-311+G(2d) results
		$\stackrel{\sim}{\sim}$		~ .	_		\sim	ഗ
3		2		>	>			()
4	Z							\sim
7								Ų
1								-
34E.5	and What is	#33.554g	1,000	and analysis	23/8/5/-3	2000 100		



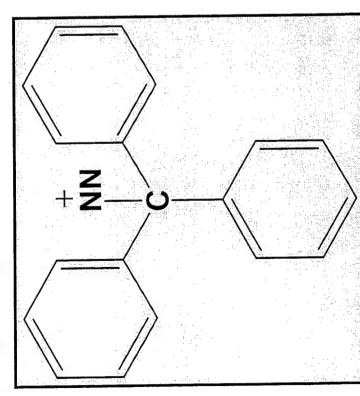




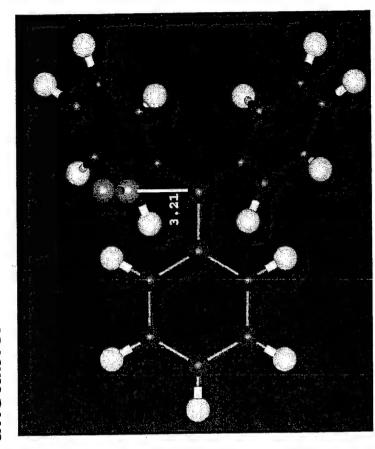
Identifying Precursors for New Polynitrogens



This ion has been suggested as a useful precursor to new polynitrogen molecules...



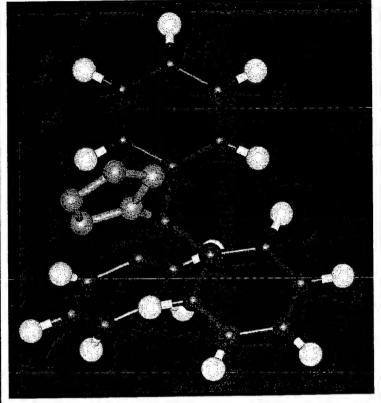
... but calculations predict it to be unstable.

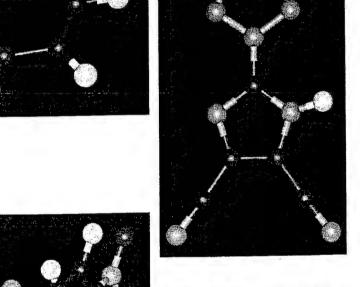


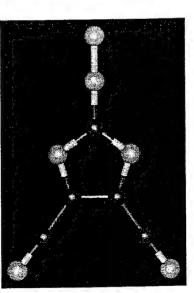
Computational requirements: ~10,000 CPU-hours, 1200 MW on IBM SP/P3 at ASC

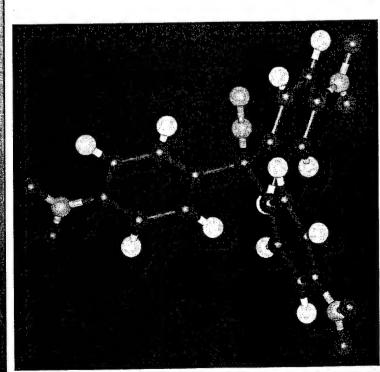
Other Potential Polynitrogen Precursors Being Investigated













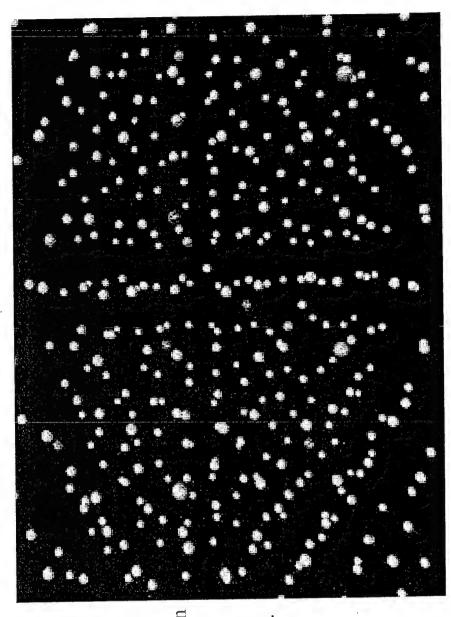




6.25% B atoms in solid para-H₂

Previous key results

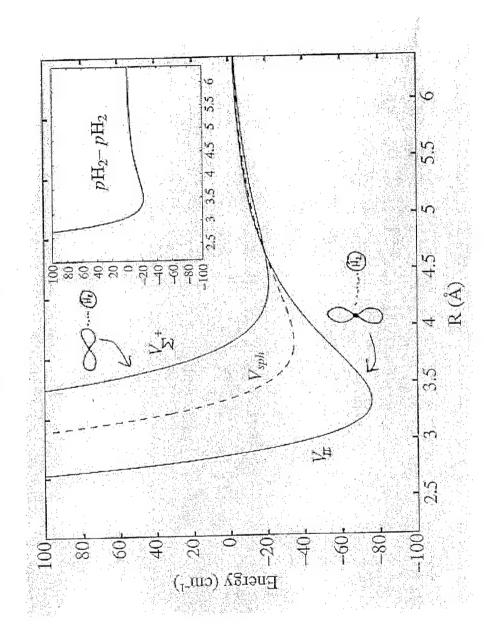
- 1. In sH₂, B atoms more stable than Li atoms
- 2. No recombination of B atoms seen at concentrations up to 6.25%.
- 3. "Forced" recombination of B atoms does not trigger phase separation.





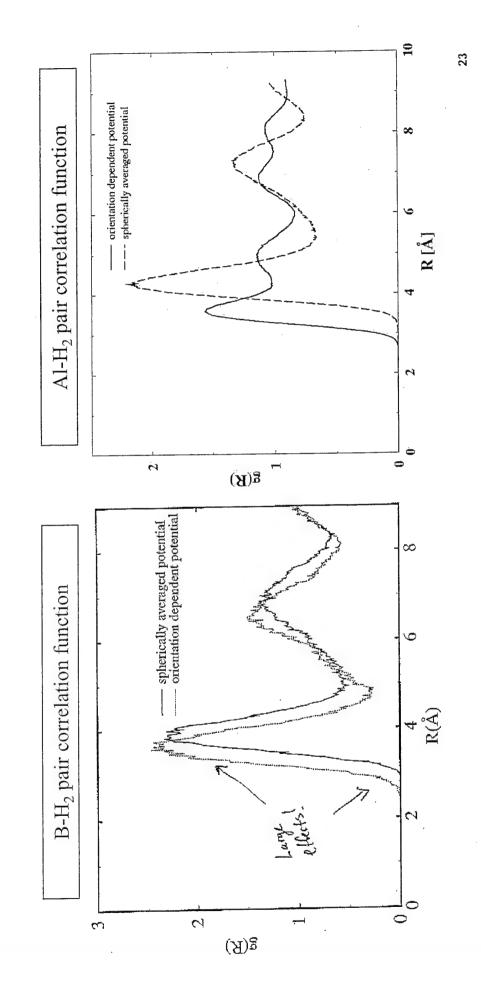


How important is the orientational dependence of B-H₂ (Al-H₂) interactions in B/sH_2 (Al/sH₂)?













B-H₂ and Al-H₂ interaction energies (cm⁻¹)

\ \^\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	3,33)	20	237	
$<$ VALH $_2$ >	-263.41 (17.3.	-273.86	-179:52
<v<sub>B-H2></v<sub>	546.72 (1.92) =263.41 (3.33)	443,32 (4.92) -177,37 (4.26)	-538:49 (6.06) -273:86 (2.37	439.88 (3.56) -179,52 (1.90)
	-546.7	-443.3	-238.7	-439.8
	Orientation dependent	Spherically averaged	Orientation dependent	Spherically averaged
		Impurity no defect	Ímpurity	& defect

Krumrine, J.R., Jang, S., Alexander, M.H., and Voth, G.A.: J. Chem. Phys. 113 (2000) 9079

Mirijanian, D.T., Alexander, M.H., and Voth, G.A.: To be published

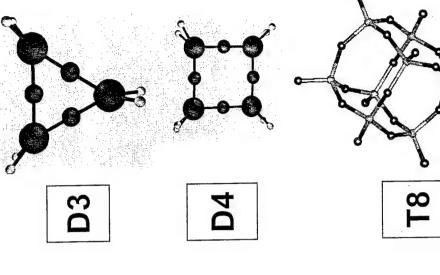
Key steps

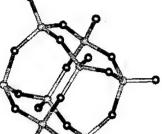
Mechanism of formation

- 1. Hydrolysis of RSiX₃ (R=H,CH₃,t-butyl,etc.; X=Cl) $RSiCl_2OH + H_2O \rightarrow RSiCl(OH)_2 + HCl$ $RSiCl_3 + H_2O \rightarrow RSiCl_2OH + HCI$ $RSiCl(OH)_2 + H_2O \rightarrow RSi(OH)_3$
- $2 \text{ RSi(OH)}_3 \rightarrow \text{R(OH)}_2 \text{SiOSi(OH)}_2 \text{R} + \text{H}_2 \text{O}$ 2. Condensation of RSi(OH)₃ to disiloxane
- $RSi(OH)_3 + R(OH)_2SiOSi(OH)_2R \rightarrow D_3 + 2H_2O$ 3. Condensation of disiloxane to D_3,D_4

[3+1]: RSi(OH)₃ + R(OH)₂SiOSi(OH)₂R \rightarrow D₄ + 2H₂O Ring.Expansion: $RSi(OH)_3 + D_3 \rightarrow D_4 + H_2O$ [2+2]: $2R(OH)_2SiOSi(OH)_2R \rightarrow D_4 + 2H_2O$

4. Condensation of D₃, D₄ to POSS (in progress) $2D_4 \rightarrow T_8 + 4H_2O$









Mechanism of formation: role of solvent (H2O) & substituents (R)

e L	Energy barrier (kcal/mol)	(kcal/mol)	
	HF/6-31/G*	MP2/6-31G*	
	30:4 (16:7)	10.9 (-9.3)	
Ne	28.2 (14.7)	7.7 (-13.3)	
∂B U	34.3 (24.9)	9.8 (-9.3)	
	31.1 (18.2)	7.9 (-16.4)	

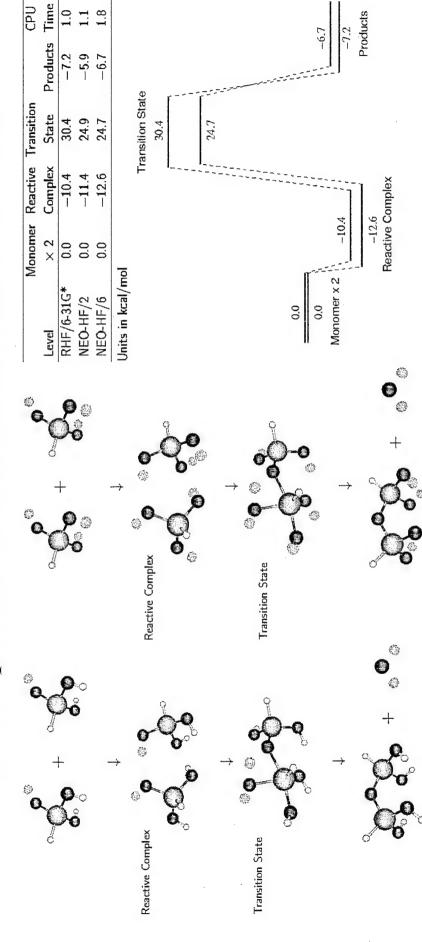
TS for the condensation of RS(OH)₃ catalyzed by a water (1356) (HF/6-31G*) (

Kudo, T., Gordon, M.S. J. Am. Chem. Soc., 120, 11432 (1998) Kudo, T., Gordon, M.S. J. Phys. Chem. A, 104, 4058 (2000)





Nuclear quantum effects in condensation reactions



Hammes-Schiffer, S.: J. Phys. Chem. A 102 (1998), 10443

Webb,, S.P., Agarwal, P.K., and Hammes-Schiffer, S.: J. Phys. Chem. B, 104(2000), 888

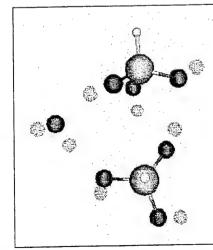
Webb, S.P. and Hammes-Schiffer, S... J. Chem. Phys. 113 (2000), 5214

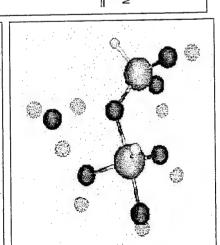




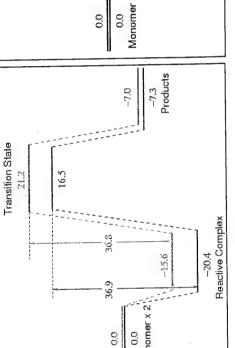
Nuclear quantum effects in water-catalyzed condensation reactions

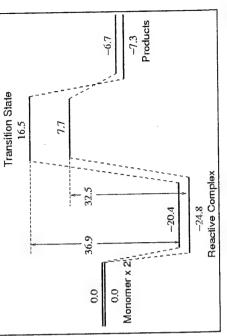
 $2 \times HSi(OH)_3 + H_2O \rightarrow H(OH)_2Si-O-Si(OH)_2H + 2H_2O$





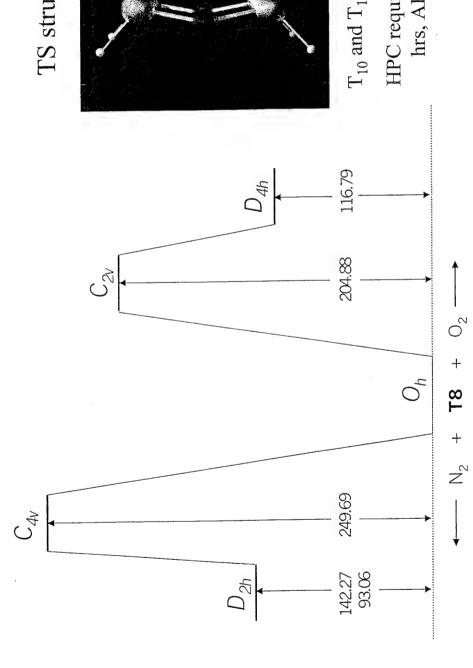
	Reactive	Transition		CPU
	Complex	State	Products	Time
RHF/6-31G*	-20.4	16.5	-7.3	1.0
NHF/6-31G*/ZPE	-15.6	21.2	-7.0	
VEO/HF/4	-23.0	7.2	-5.9	1.1
VEO/HF/8	-24.8	7.7	-6.7	1.8

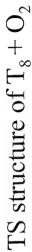


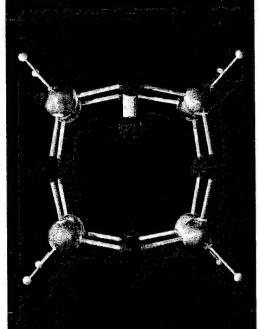




Molecular "sieves": preferential capture N₂ vs. O₂?







T₁₀ and T₁₂ calculations in progress HPC requirements: ~50,000 nodehrs, AHPCRC T3E, 256 GB

RESULTS - NLO

B3LYP S₀-T₁ Excitation Energies (in eV)

System	6-31G(d)	Error	Exp
Porphyrin (1 ³ B _{2u})	1.42	0.16	1.58^{a}
Zinc Porphyrin (1 ³ B ₁ u)	1.65	0.07	1.72b
Tetraphenylporphyrin (1 ³ B ₁)	1.31	0.14	1.45 ^c
Zinc Tetraphenylporphyrin(1 ³ B ₁)	1.53	90.0	1.59d
Zinc Phthalocyanine (1 ³ B _{2u})	1.05	80.0	1.13e
Zinc Tetrabenzporphyrin (1 ³ B _{1u})	1.41	0.16	1.57^{f}
Phthalocyanine (1^3B_{1u})	1.18	90.0	1.248
Mean Error		0.10	

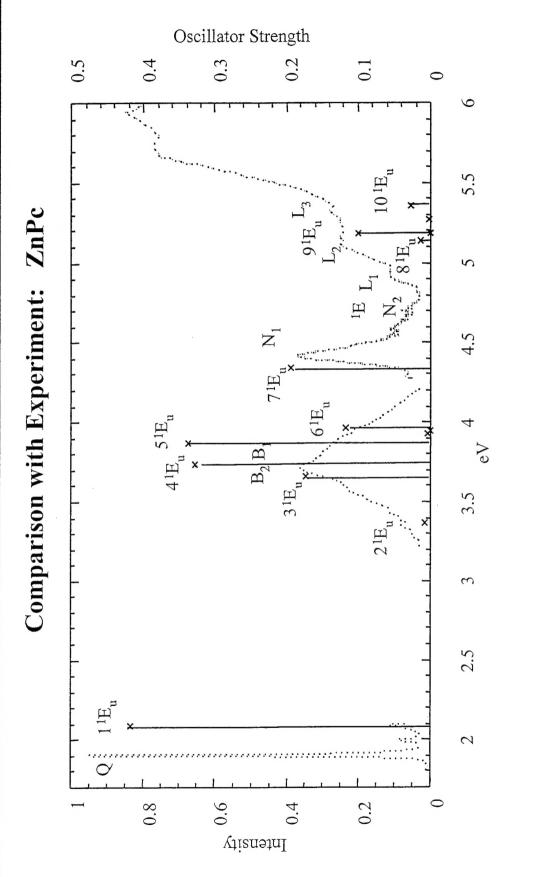
Gouterman, J. Mol. Spectrosc. 1971, 39, 421 (octane at 77 K) McVie et al., J. Chem. Soc. Faraday Trans. II 1978, 74, ether to ethanol at 77 K) eVincett et al., K. E. J. Chem. Phys. 1971, 55, 4131. (1-chloronapthalene at 77 K) Bajema, Khalil, J. Mol. Spectrosc. 1974, 53, 88. (EPA at 77 K) dWalters et al., J. Phys. Chem. 1995, 99, 1166.(1:1 mixture of ^aGouterman, Khalil, J. Mol. Spectrosc. 1974, 53, 88. (EPA (5:5:2) mixture of ethyl ether to isopentane to ethanol and 50% ethyl iodide at 77 K) bGradyushko, Tsvirko, Opt. Spectrosc. 1971, 31, 291.(EPA at 77 K) Couterman, 1870 (1-chloronapthalene at 77 K)

27 TO E		*****	1200	-
L'AND MAN	The state of	Tree nav		200
A TOTAL	~	1		
COLUMN TO A STATE OF	~			100
	200	300		
	1			198
	NO.	1		25/25
~			1	
7.12	200	1		
-	725	100	-54	
-	192		SERVE	
•		THE W		
Carrier Cont		V. MEZA NO	NOTE OF	1
A. 264	No.	13	3.787	
O	1980			24
S. A.	100 2 W	16.		
	The said	AL PARTY OF	Der	2
		100 (200)	CEL SA
VA SHE	7.Y2.	20		della
27.00	1	13 6	1	
100	10	100	120	1
The same	Sec.	200		1
	2000			And
	34 48	(NEW)	1170	Circles .
1			1336	19:39
100		1 11 1-0	N. C.	1.70
120		The second	Marie Contract	1
15		15/11/20	CV-	76
2 8 19	1		1	Alexander of
A STATE OF	1	The same of	13500	1
V.	-	13	1 C	· ·
>	1	The state of the s	1	1
100	Dett.	Jane C.	The Cone	1.50
21	6.328°		1340)
0	The same of the sa	1	1 Sul	1
Jan order	2.7	YUT	1	1
N. Janes	Car		300	1
The state of	1200	STATE OF THE PARTY OF	Section 1	15.75
	1	A STATE OF THE STA	100	100
1	U	1	1 1 1	P. S.
1442 (1 T		WHAT S	-C	2
170	1	Carlon To Care	Tarana and	1
1	Rose Co	12.3	18.6	-1,313
T	1000	WA.	grant.	440
ت	201	122	(D)	-
MONTH	19 19 19		100 m	4 4
	A STATE	A. 42. 25		155
200	12	200	3 7.	-
Const.	并图1 50	F Short of	SHAP A	3
100	H. S.	4.3	1858	416
13.50	17. 17. 6	7.2015	10.5	1
~			200	13.
	150	25	124 3	1
1:30	Cart of the	Setting	196(2)	1. g 40
2001			1	200
3	SELECTION OF	3000	Green and	1110
	100		17.5 20.7	
	· · ·) _ (L	1	
_ Q.	4	3 - <u>ር</u>	3	\sim
- 0	<u> </u>	}		'n
Ļ	<u></u>	1 T) 2 2	ì
ر د د	1 - 2	ohte ohte	1 6	, T
ار 1	14 S	ochte Ichte		,
20hre	2017	achte	Dhys	,
Pachie	Dachte	Pachte	7.40.1	,
Pachle	Dachte	Pachte	1 05.00	, T :
1 Pachte	1 Dachte	i Lacino I Pachte	7 Dhv.	, d. 1 11.y
d Pachte	J Dachte	d Pachte	7. Dhees	
nd Pachte	ad Dachte	ad Pachte	9340.1	
ind Pachie	nd Pachte	ind Pachte	P. T. Dhave	
and Pachte	and Pachte	and Pachte	P. T. Dheve	
and Pachte	and Pachte	and Pachte	P. T. Dhees	
and Pachle	and Pachte	., and Pachte	D. T. Dhess	
F and Pachle	I and Pachte	I. and Pachte	ar P. T. Dhee	これにいる
V and Pachte	V and Pachte	Z. and Pachte	ter D. I Dhee	
N and Pachte	N and Pachte	N and Pachte	otter D. T. Dhens	
N and Pachile	N and Pachte	N and Pachte	hter P. I Dhyn	
2 N and Pachfe	N and Pachte	. I. and Pachte	shier P T Dhys	
P. N. and Pachfe	P. N. and Paclate	P. N. and Pachte	Solution D. T. Diving	acmer; N., my
P N and Pachte	P. N. and Pachte	P. N. and Pachte	Schlar D. 1 Dhus	action uy
. P. N. and Pachte	P N and Pachte	. P. N. and Pachte	Dochter P. T. Dhwe	action, Iv., J., III
v P N and Pachte	V. P. M. and Pachte	V. P. N. and Pachte	Dochter P. I Dhwe	1 delicit 10., 4. 1 my
ty P N and Pachte	W. P. M. and Pachte	y, r. r., and Fachte	1 Dochter P. I. Dhye	
lay P N and Pachte	lay P N and Pachte	lay P N and Pachte	d Dochter D. T. Dhwe	
Day P. N. and Pachte	Day P. M. and Pachte	Day P. N. and Pachte	nd Dochter D. 1 Dhys	
Dav P. N. and Pachte	Day P M and Pachte	Day, P. M. and Pachte	and Dochter D. L. Dhye	alid Lacifici, iv. 1 mys
Day P N and Pachte	Day P N and Pachte	Day P N and Pachte	and Dachter D. 1 Dhye	
Day P N and Pachte	Day P N and Pachte	Day P. N. and Pachte	and Dachter B. I. Dhwe	and action, as a my
Dav P. N. and Pachte	Day D M and Pachte	Day P N and Pachte	and Dachter D. I. Dlave	N. Alle Lacillett IV., v. I uye
A Dav P N and Pachle	A Dav. P. N. and Pachte	A. Dav. P. N. and Pachte	A and Dachter P. 1 Dlaws	A. aliga action, i., a. tanyo
A Day P N and Pachle	A Day P N and Pachte	A. Dav. P. N. and Pachte	A and Pachier D. I. Divis	A. ald lacille, i., v. t liye
A Day P N and Pachte	A Day P N and Pachte	A Dav P N and Pachte	A and Dachter P. 1 Dlage	
. A. Dav P. N. and Pachle	A Day P N and Pachte	A Day P N and Pachte	A and Dochter P. I Dlaws	יילי שום בסכווכני, יייד וואי
A Day P N and Pachte	C A Day P N and Paclite	K. A. Dav P N and Pachte	7 A and Dachter D. I. Dlaws	
K A Dav P N and Pachle	K. A. Dav. P. N. and Pachte	K. A. Day, P. T., and Pachte	V A and Dochter D Dlave	N.A. alid Lacinci, 18, 5, 1 my
K A Day P N and Pachre	V A Day P N and Pachte	K A Day P N and Pachte	V A shd Dachter D. I. Dhwe	, N. A. Alla Lacinci, iv. 1 my
K A Dav P N and Pachte	K A Day P N and Pachte	K A Day P N and Pachte	V A and Dochter P. L. Dhwe	I, N. A. alle Lacinoi, IV., v. I IIV.
n K. A. Dav P. N. and Pachte	n V A Day P N and Pachte	$\Gamma_{i}, \Gamma_{i}, $	n V A and Dachter P T Dhwe	H, N. A. alid Lacinot, IV, v. Liny
on K. A. Dav. P. N. and Pachte	an K A Day P N and Pachte	The Karling of the State of the	in V A and Dachter D. I. Dhwe	on, n. T. and Lacinot, 18, c. t my
en K. A. Dav P. N. and Pachte	on V A Day P N and Pachte	ren K. A. Dav. P. N. and Pachte	on V A and Dochter P. T. Dhwe	Vell, N. A. allu Lacinci, IV., J. Luye
ven K. A. Dav. P. N. and Pachte	ven K. A. Day, P. N. and Pachte	ven K. A. Dav. P. N. and Pachte	Jon V A and Dachter D. I Dhwe	Yell, N. A. alid Lacinot, IV., J. Linyo
iven K. A. Dav P. N. and Pachte	wen K A Day P N and Pachte	Iven K. A. Dav P. N. and Pachte	wan V A and Dachdar D. I. Dhwe	TYCH, N. M. ALIDA LACHICL, IV., G. T. HYC
nven K. A. Dav P. N. and Pachte	wen K A Day P N and Pachte	uyen K A Day P N and Pachte	wen V A and Dechter D. I Dhwe	יניין, ואיילה, מווען מכוווטן, ואי, מייד וואי
miven K A Dav P N and Pachte	niven K Δ hav P N and Pachte	buyon, iv. iv., Duy, i.e.i.,, ama i achic	Edver Transfer Development Devices	פעיסוו, זאי להי מוועד מכוונכן, זאי מי ד חיי
Tonven K. A. Dav. P. N. and Pachte	Tanyan K A Day D N and Dachte	(Sulven, N. 13.), Laft, and Lachte	Sulver I A and Docktor P. I Dhys	egayon, n. r. and racino, iv, v. r nyo
Jones K. A. Dav. P. N. and Pachte	Tennen K A Day P N and Pachte	Jouven K. A. Day, P. N. and Pachte	Tanyan V A and Dochter D I Dlyve	Agayon, N. A. and Lacinet, 18, 0, 1 mys
Nonven K.A. Dav. P. N. and Pachte	Names K Δ Day P N and Pachte	Nouven K. A. Day, P. M. and Pachte	Manyan I A and Docktor D. I Dhys	INGUYOH, N. A. AHU LACHIOL, IV., C. LHYO
Notiven K A Day P N and Pachte	Nanyen K A Day P N and Pachte	Nouven K. A. Day P. N. and Pachte	Menusan V. A. and Dochter D. T. Dhys	Lyguyon, N. A. and Lacinci, IV. v. 1 nyo
Nonven K. A. Dav. P. N. and Pachte	$N_{miven} K \Delta \Gamma_{ax} P N$ and Pachte	Nouven K. A. Day P. N. and Pachter R1 Phys. Chem. 404 (2000) 4755	Manyan V. A. and Dochter, D. T. Dhye	INGUYOH, N. A. AHUL ACHIOL, IN., J. 1 HYG
Notiven K A Day P N and Pachte	Nonven K A Day P N and Pachte	Nouven K A Day P N and Pachte	Name I A and Docktor D I Dlaye	Nguyell, N. A. aliu acilici, IV., v. 1 nye
Norven K A Day P N and Pachte	New Year K A Day P N and Pachte	Nouven K. A. Dav. P. N. and Pachte	New V A and Dachter D. T. Dlave	Nguyon, n. A. and a concitation and
Nouven K. A. Dav. P. N. and Pachte	New York A Day P. V. and Pachte	Nouven K. A. Day P. N. and Pachte	Now and Vandance Days	INGUICHT, IN. THE ANTIOURISM, ST. LIDS
Nouven K. A. Day P. N. and Pachte	Newton K A Day P M and Pachte	Nouven K.A. Day, P. N. and Pachte	Nowe V A and Dochtar D. T. Dlave	Nguyen, N. A. and action, IV., J. 1 nye

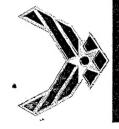
HPC Requirements: ~100,000 CPU hours, on SGI O2K + IBM SP3 + SGI O2K @ ASC



RESULTS - NLO







SUMMARY



High Energy Density Matter

- High-nitrogen/polynitrogen compounds are more energetic than hydrazine.
- Trityldiazonium cation is not a stable polynitrogen precursor.
- Inclusion of anisotropic interactions of B, Al atoms in sH2 predict greater stability than spherical interaction model.

Polyhedral Oligomeric Silsesquioxanes (POSS)

- Proton transfer reactions for hydrolysis and condensation are catalyzed by
- Alkyl substituents (R) in RSiX₃ have minor effects on hydrolysis and condensation reaction barriers.
- Nuclear quantum effects are important in proton transfer reactions -- lower barriers by >5 kcal/mol.
- T_8 is too small to encapsulate N_2 or O_2 .



SUMMARY (cont.)



NLO materials

- Time-dependent density functional theory accurately predicts NLA in porphyrins.
- Computed triplet-triplet excitation energies within 0.1-0.4 eV of experiment
- Computed singlet-triplet excitation energies within 0.1-0.2 eV of experiment
- Computed ionization potentials accurate within 0.1 eV of experiment



ACKNOWLEDGEMENTS



POSS: Takako Kudo, Shawn Phillips, Simon Webb, Frank Feher, Joe Lichtenhan

HEDM: Millard Alexander, Jennifer Krumrine, Soomin Jang, Jeff Mills, Jeff Sheehy, Don Thompson, Dan Sorescu

NLO: Kiet Nguyen, Paul Day

GAMESS: Graham Fletcher

MSRCs, DCs: ASC, ARL, ERDC, NAVO, MHPCC, AHPCRC, ARSC, AFFTC

CHSSI funding (CCM-2, CCM-4, MBD-01)